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INTERMOLECULAR INTERACTION OF GLYCYRRHIZIN WITH CHOLESTEROL

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Abstract. Glycyrrhizin (glycyrrhizic acid, 3-O-β-D-glucuronopyranosyl-(1→2)-O-β-D-glucuronopyranoside of 18β-glycyrrhetinic acid, GA) is the dominant triterpene saponin from licorice roots *Glycyrrhiza glabra* L. and *Glycyrrhiza uralensis* Fisch. (Fabaceae) .[1]

Some biological properties of triterpene and steroid saponins explain their molecular complexation with sterols.[1, 2] GA increases permeability and reduces the elastic modulus of cell membranes.[3] On the other hand, recent spectrophotometric titration did not confirm the complexation of monoammonium salt of GA (GC) with cholesterol (Chol) and 1,2-dipalmitoylphosphatidylcholine.[4]

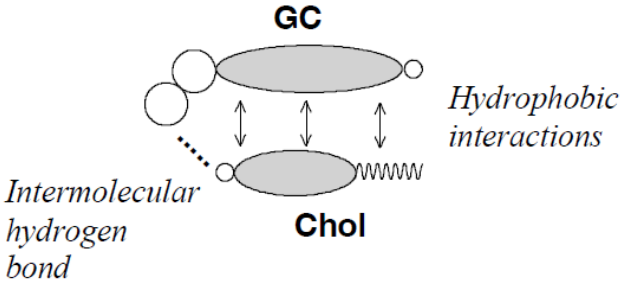

Figure 1. Schematic representation of the possible orientation of GC and Chol molecules during their intermolecular interaction

In order to consider the possibility of complexation of GA and GC with Chol in various media, we studied their intermolecular interaction in aqueous isopropyl alcohol by NMR, IR, and UV spectroscopy. The 1 : 1 molecular complex of GC with cholesterol was obtained in 80% aqueous isopropyl alcohol for the first time.

The intermolecular interaction of GC with Chol was studied by UV spectroscopy. As the GC concentration increases (at constant Chol concentration), the optical density of their solutions increases (hyperchromic effect). The absorption maximum of the solutions increases (bathochromic shift) from 237 to 250 nm.

The formation of an intermolecular hydrogen bond between OH group at C-3 of Chol and C=O group of terminal glucuronic acid residue in the carbohydrate part of GC (C^3–O–H…O=$C^{6''}$) and hydrophobic contacts were confirmed by ^{13}C NMR and ATR FT-IR spectroscopy (Fig. 1).

References

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